Comparison of Nucleon Cross Section Parameterization Methods for Medium and High Energies

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Abstract

Several methods for the parameterization of nucleon reaction and elastic scattering cross section at medium and high energies were tested and compared with each other, with medium-energy optical model calculations, and with evaluated nuclear data libraries. It is shown that the methods are generally consistent for nucleon reaction cross sections over a wide energy range for masses from carbon to lead.

Introduction

This study had its origins in the effort to provide a medium and high energy cross section definition package for LAHET3 and MCNPX[1],[2]. The FLUKA'96[3] routines were made available along with the high energy generator for inclusion in LAHET3. Subsequently, methods being developed by NASA[4],[5] were made available, as were those from the CROSEC code[6]. Additional contributions were provided by recent work with a global medium energy optical model[7] and the development of evaluated neutron data libraries to 150 MeV[8]. The study has been confined to nucleon cross sections, since only for these are there a multiplicity of methods available for comparison.

The objectives of the study have been to (1) test consistency of methods, (2) indicate areas for improvement of methods and data evaluations, (3) detect limitations in coding, modeling, and evaluation, (4) provide assistance in documentation and quality assurance, and (5) offer guidance for construction of composite methods. In some sense, it should provide some indication of what "state of the art" might mean in this area.

The Methods Considered

The cross section definition routines from the FLUKA'96 code[3] are a composite of methods which will not be detailed in this paper. However, they do provide treatment of all hadrons and include the high energy method of Moehring[9]. Integrated as they are with the code structure of FLUKA, the necessary subroutines are not readily available as a stand-alone package; they require the use of input from data files. Addition code for ^{2}H targets is available but not included in this study. Results obtained from the FLUKA methods are designated by "**FLUKA**" in the following discussion.

The method of Barashenkov and Polanski ("**B & P**") is discussed in some detail in the next section; it provides cross sections for nucleons and pions. The code package is of modest size and easily implemented; input data files are required.

The NASA method ("**NASA**" below) provides reaction cross sections for nucleons and ions through a universal parameterization[4],[5]; it is available as short, simple code. A similar treatment for elastic scattering cross sections is under development, but not included in the present study.

The method of Wellisch and Axen ("**W & A**") provides an easily implemented phenomenological parameterization for proton reaction cross sections only. The original publication[10] included erroneous parameter values. The corrected values[11] are documented in reference [12] along with an extension to targets with $A < 12$. Some results using this method have been published previously[1].

The optical model calculations[7] shown in this study were made for 9 mass values (^{12}C, ^{16}O, ^{27}Al, ^{40}Ca, ^{56}Fe, ^{81}Br, ^{107}Ag, ^{138}Ba, and ^{208}Pb) and 20 energies from 50 MeV to 400 MeV. They are also used as an interpolation table to provide nucleon reaction and elastic scattering cross sections in the range 50 MeV $\leq E \leq$ 400 MeV for targets with $12 \leq A \leq 208$. Results so obtained are designated "**DGM**" in the discussion below. The nucleon elastic scattering cross section method has been implemented and tested in LAHET3[13] and MCNPX[14].

The Method of Barashenkov and Polanski

A number of methods have been employed to calculate dependence of cross sections *vs.* energy. At high energies $E > 10$ GeV, Regge theory is used which allows one to describe simultaneously the cross sections for several types of particles using the same set of parameters [15].

At medium energies, where the projectile de Brogle wave length is significantly smaller than the size of the target nucleus, an optical model based on a solution of the Schrödinger equation with a phenomenological potential was used[16],[17],[18]. The parameters of this model have been fitted to obtain the best agreement of calculated and experimental data. The experimental data were obtained from the compilations of Barashenkov [19]. The medium energy region has been divided into separate intervals showing characteristic behavior of cross sections. (For example, the region near the minimum of nucleon cross sections at energy about 200 MeV, the resonance region near 180 MeV in the case of pion-nucleus cross sections, the interval of smooth cross section alterations at energy above 1 GeV). A set of parameters has been defined for each interval.

At lower energies a phenomenological approximation[19],[20],[21] for the cross sections was used:

$$\sigma(A,Z,E) = \pi[r_0 A^{1/3} + \lambda(A,E)]^2[1 - V(A,Z)/E_c]f(E)\phi(A)^{\alpha(E)}$$

where V is the Coulomb barrier , λ and E are the de Brogle wave length and the kinetic energy of the projectile in the center of mass system. A and Z are the target nucleus mass and charge numbers. The functions $f(E)$, $\phi(A)$ are determined by the sums:

$$\Sigma_i \alpha_i E^{\beta_i} \quad \text{and} \quad \Sigma_i a_i A^{b_i}$$

with constant coefficients; $\phi(A) \rightarrow A$,
; $\alpha(E) \rightarrow const$ as the projectile energy increases.

Below 20 MeV the neutron cross section evaluations were taken from the Abagian evaluations [22].

The total, nonelastic and elastic cross sections have been evaluated for neutrons, protons and pions incident on the following isotopes with mass numbers:

4.00	9.01	12.00	14.00	16.00	23.00	26.98	40.08
47.90	55.85	63.55	79.90	95.94	112.40	118.69	137.34
183.85	207.19	238.03					

The proton-nucleus and neutron-nucleus evaluated cross sections have been calculated for the following energies (in MeV):

14	15	16	17	18	19	20	22
25	27	30	33	35	37	40	45
50	55	60	65	70	80	90	100
120	140	150	160	180	200	250	300
350	400	500	600	700	800	900	1000
1500	2000	3000	5000	7000	10000	20000	50000
100000	500000	1000000					

The result of the evaluations is saved as a BARPOL.DAT file. The hadron-nucleus cross sections are then calculated by means of an interpolation of the tabulated values for other targets at other energies using the CROSEC code[23],[24],[6]. Some parts of this code are used as subroutines in the Dubna High Energy Transport Code[25].

method	projectile	type	mean ratio	RMS deviation
FLUKA	proton	elastic	0.923	0.201
FLUKA	neutron	elastic	1.051	0.164
B & P	proton	elastic	0.939	0.270
B & P	neutron	elastic	0.987	0.160
NASA	proton	reaction	1.012	4.97E-2
NASA	neutron	reaction	0.995	4.35E-2
FLUKA	proton	reaction	0.998	3.77E-2
FLUKA	neutron	reaction	0.987	4.60E-2
B & P	proton	reaction	0.985	4.45E-2
B & P	neutron	reaction	0.996	4.67E-2
W & A	proton	reaction	1.016	4.03E-2

Table 1: Comparison with DGM optical model calculations: 9 masses, A=12 to 208, 20 energies 50 MeV to 400 MeV.

Comparisons with Optical Model Calculations and MCNP Evaluated 150 MeV Neutron Data Libraries

The optical model calculations[13] used for this analysis are the reactions and elastic scattering cross sections for neutrons and protons, for 9 masses (^{12}C, ^{16}O, ^{27}Al, ^{40}Ca, ^{56}Fe, ^{81}Br, ^{107}Ag, ^{138}Ba, and ^{208}Pb) and 20 energies (50, 60, 70, 80, 90, 100, 110, 120, 140, 160, 180, 200, 225, 250, 275, 300, 325, 350, 375, and 400 MeV). In table 1, each method is compared as the mean ratio to these 180 optical model calculations and as

method	projectile	type	mean ratio	RMS deviation
FLUKA	neutron	elastic	1.063	0.125
B & P	neutron	elastic	1.006	6.93E-2
NASA	neutron	reaction	1.002	5.50E-2
FLUKA	neutron	reaction	0.977	6.61E-2
B & P	neutron	reaction	0.970	8.16E-2

Table 2: Comparison with MCNPX data files. Total number of points: 4265.

the root mean square deviation. Over this range of mass and energy, all the methods are remarkably consistent for both proton and neutron reaction cross sections; no method shows more 1.6% mean deviation or more than 5% RMS deviation.

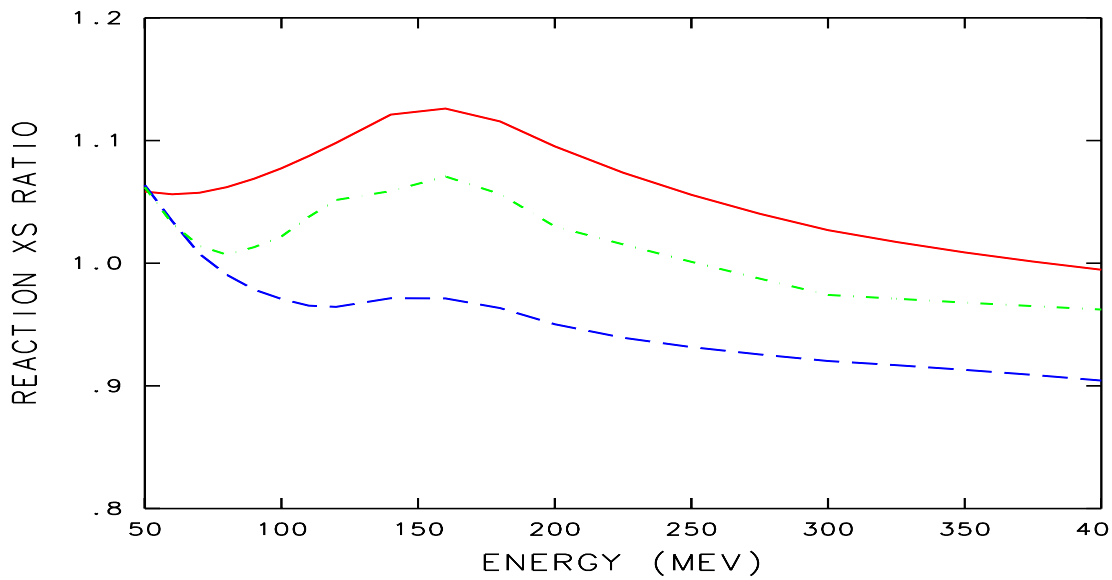

Figure 1: Comparison to optical model calculations for ^{56}Fe. FLUKA: long dash line; NASA: solid line; B & P: short dash line.

A second comparison was made with evaluated data from 150 MeV and 100 MeV MCNP neutron data libraries[8]. The neutron reaction and elastic scattering data for these comparisons were extracted from the 29 following 150 MeV MCNP neutron libraries: ^{2}H, ^{12}C, ^{14}N, ^{16}O, ^{27}Al, ^{28}Si, ^{29}Si, ^{30}Si, ^{40}Ca, ^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr, ^{54}Fe, ^{56}Fe, ^{57}Fe, ^{58}Fe, ^{58}Ni, ^{60}Ni, ^{61}Ni, ^{62}Ni, ^{64}Ni, ^{182}W, ^{183}W, ^{184}W, ^{186}W, ^{206}Pb, ^{207}Pb, ^{208}Pb and the two following 100 MeV neutron libraries: ^{9}Be, ^{238}U. The total number of data values for comparison is 4265 in each case. In table 2, the same computations as above are shown. In this lower energy range, the variability among the models is rather larger for reaction cross sections, and smaller for the elastic cross sections.

A set of color Postscript plots illustrating these comparisons are available for download[26]. Examples of the plots are shown in figures 1 and 2. The variation among the different methods and the evaluated data libraries is most easily understood with the graphical results.

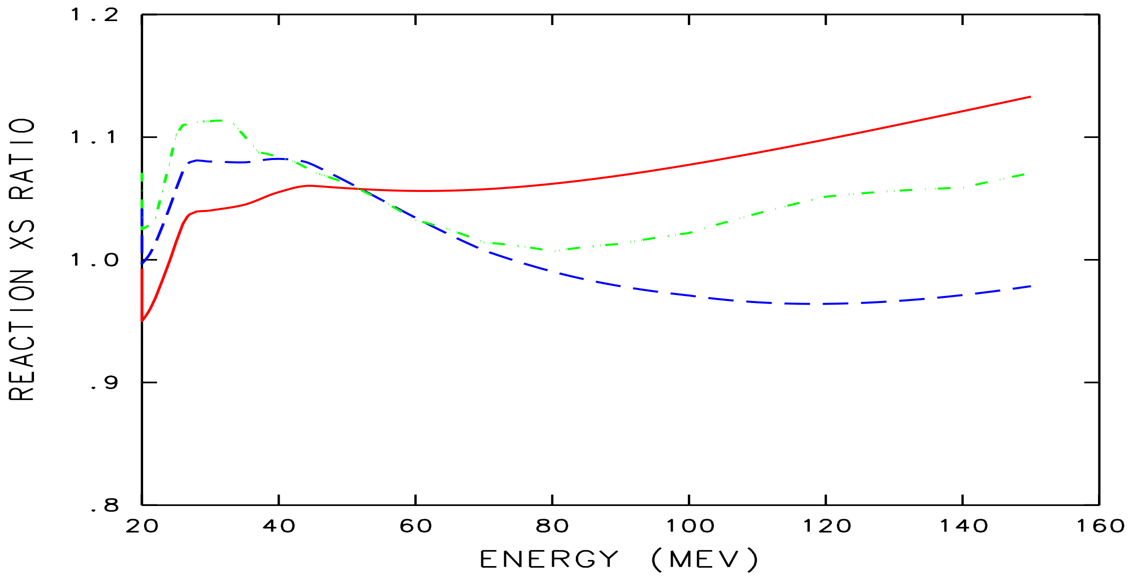

Figure 2: Comparison to MCNPX data library for ^{56}Fe. FLUKA: long dash line; NASA: solid line; B & P: short dash line.

Comparison to Experimental Data

Compilations of neutron and proton reaction and elastic scattering cross sections were extracted from the files of reference [19]. The graphical comparison of the model calculations with experimental data is shown in the rather large plot files available for download[26]. These plots, although qualitative, are the more important part of the comparison. They may be examined for discontinuities, interpolation artifacts and other undesirable features. (Such characteristics may be observed in the the 150 MeV evaluated data libraries, as well.)

The extracted experimental data were also used for a statistical comparison with the models, with the optical model calculations ("**DGM**") discussed above applied as an interpolation table for 50 MeV $\leq$ E $\leq$ 400 MeV and 12 $\geq$ A $\geq$ 208. The neutron reaction cross section comparison is shown in table 3, for reduced χ^2, and table 4,

Range of data				DGM		FLUKA		B & P		NASA	
Z_{min}	Z_{max}	E_{min}	E_{max}	n	χ^2	n	χ^2	n	χ^2	n	χ^2
2	100	0.0	10 TeV	40	2.99	493	6.40	491	7.48	355	5.80
6	82	20 MeV	50 MeV	0		42	1.43	42	1.36	42	1.17
6	82	50 MeV	400 MeV	40	2.99	40	1.93	40	2.92	40	6.22
6	82	400 MeV	10 GeV	0		147	3.40	147	3.19	147	3.93

Table 3: Neutron reaction cross section comparison to experimental data: reduced χ^2.

Range of data				DGM		FLUKA		B & P		NASA	
Z_{min}	Z_{max}	E_{min}	E_{max}	n	%	n	%	n	%	n	%
2	100	0.0	10 TeV	40	9.04	493	9.70	491	10.43	355	9.37
6	82	20 MeV	50 MeV	0		42	6.23	42	5.70	42	5.45
6	82	50 MeV	400 MeV	40	9.04	40	8.84	40	8.63	40	9.16
6	82	400 MeV	10 GeV	0		147	11.10	147	10.44	147	10.29

Table 4: Neutron reaction cross section comparison to experimental data: RMS deviation (%).

for RMS deviation. Similar comparisons for proton reaction cross section data are shown in tables 5 and 6. In these tables, n represents the number of experimental data points at which the particular method could be applied. The range $12 \geq A \geq 208$ is emphasized since all methods are valid for these masses; the first line in each table represents a comparison to *all* available experimental data.

Two data points, which contributed more than 90 % of the calculated overall χ^2, were removed from the neutron data; the proton data file was unedited, although perhaps some evaluation of individual data points should be performed. However, the extent of the data is sufficiently broad that the statistical comparison should be meaningful.

A similar analysis for the elastic scattering data is not included here, since the extent of the data is much more limited, and a statistical comparison is meaningful only for a few elements. (The proton elastic data are largely restricted to ^{4}He and ^{27}Al.) The comparison should be made on the *total* cross section, but the necessary data have not yet been extracted from the files of reference [19]. Generally, however, the observed RMS deviation from the data files is about 30%.

Range of data				DGM		FLUKA		B & P		NASA		W & A	
Z_{min}	Z_{max}	E_{min}	E_{max}	n	χ^2	n	χ^2	n	χ^2	n	χ^2	n	χ^2
2	100	0.0	10 TeV	128	5.04	1598	8.43	1429	8.07	1602	15.82	1602	14.42
6	82	0.0	20 MeV	0		194	18.64	55	6.80	194	43.51	194	27.66
6	82	20 MeV	50 MeV	0		374	4.77	374	7.94	374	3.70	374	6.99
6	82	50 MeV	400 MeV	128	5.04	128	7.54	128	6.57	128	10.04	128	6.15
6	82	400 MeV	10 GeV	0		449	6.41	449	10.81	449	21.34	449	8.45

Table 5: Proton reaction cross section comparison to experimental data: reduced χ^2. B & P calculations above 14 MeV.

Range of data				DGM		FLUKA		B & P		NASA		W & A	
Z_{min}	Z_{max}	E_{min}	E_{max}	n	%	n	%	n	%	n	%	n	%
2	100	0.0	10 TeV	128	10.48	1598	11.54	1429	7.71	1602	14.08	1602	12.87
6	82	0.0	20 MeV	0		194	19.53	55	9.68	194	33.07	194	26.48
6	82	20 MeV	50 MeV	0		374	4.83	374	6.47	374	4.75	374	6.50
6	82	50 MeV	400 MeV	128	10.48	128	11.51	128	9.96	128	12.88	128	11.04
6	82	400 MeV	10 GeV	0		449	5.13	449	6.09	449	5.86	449	4.78

Table 6: Proton reaction cross section comparison to experimental data: RMS deviation (%). B & P calculations above 14 MeV.

Conclusions

One immediate benefit of undertaking this study has been the completion of some improvements in models before the final results were compiled. In general, the greater benefit to a potential user of these methods will be obtained by examination of the rather large comparison plot files. One may conclude, however, that

- the methods tested indicate that the treatment of nucleon reaction cross sections is very consistent within the relatively small uncertainties discussed above, over a wide range of mass and energy;
- the treatment for nucleon elastic scattering is much less well represented, although the present study cannot supply many definitive results on this point;
- the methods which include tabulation of calculated and evaluated data at lower energy have, at least potentially, an small advantage over the methods using a pure parameterization;
- attention should be directed toward the very light and very heavy nuclei.

Future work on the CROSEC code will include a high energy treatment using the Glauber approach[27],[28],[29] for approximation of total, nonelastic and elastic cross sections and an extension of the cross section library to isotopes of Th, Pu, Am and Cm important to accelerator-driven systems technology. As noted above, the NASA methodology will be extended to a treatment of elastic scattering.

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